arXiv:1008.1174v1 [cond-mat.stat-mech] 6 Aug 2010

Phase separation transition in anti-ferromagnetically interacting particle systems

Anasuya Kundu* and P. K. Mohanty†
Theoretical Condensed Matter Physics Division,
Saha Institute of Nuclear Physics,
1/AF Bidhan Nagar, Kolkata, 700064 India.
(Dated: August 9, 2010)

One dimensional non-equilibrium systems with short-range interaction can undergo phase transitions from homogeneous states to phase separated states as interaction (ϵ) among particles is increased. One of the model systems where such transition has been observed is the extended Katz-Lebowitz-Spohn (KLS) model with ferro-magnetically interacting particles at $\epsilon = 4/5$. Here, the system remains homogeneous for small interaction strength ($\epsilon < 4/5$), and for anti-feromagnetic interactions ($\epsilon < 0$). We show that the phase separation transitions can also occur in anti-ferromagnetic systems if interaction among particles depends explicitly on the size of the block (n) they belong to. We study this transition in detail for a specific case $\epsilon = \delta/n$, where phase separation occurs for $\delta < -1$.

PACS numbers: xxx xxx

One dimensional driven diffusive systems [1, 2] have been a subject of extensive studies in recent years. Some driven diffusive models with local dynamics exhibit exotic phenomena like phase separation and phase transitions [3–8], with novel spatial correlations in their steady states, which can not be seen for systems in thermal equilibrium, with short range interactions. Since there is no general theoretical method to study non-equilibrium systems, phase transitions for them can not be inferred from any guiding principle. Few years ago a general criterion for the existence of phase separation in density-conserving one dimensional driven diffusive systems, have been proposed by using a mapping of these models to a Zero Range Process (ZRP) by Kafri *et al.* [9]. It has been suggested there, that existence of phase separation in any given model depends only on the rates (or the steady state curret J_n) at which domains of various sizes (n) exchange particles. A strong phase separation, where density fluctuations are limited to the domain boundaries, occurs for arbitrarily small densities when the steady state current J_n flowing through a block of size n vanishes for thermodynamically large blocks. Whereas a condensed phase with large density fluctuations occurs when the current

$$J_n \sim J_\infty(1 + b/n^\sigma) \qquad (1)$$

with either $\sigma < 1$ and $b > 0$ or with $\sigma = 1$ and $b > 2$. In this case phase separation occurs only for large enough densities.

This criteria [9] is based on a mapping which relates driven diffusive systems with a well known model called Zero Range Process. In ZRP, each site on a lattice (formally called boxes) can accommodate more than one particle, which are allowed to hop to the neighboring box

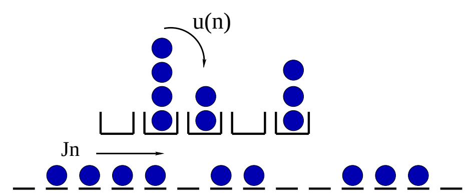

FIG. 1: A microscopic configuration of driven diffusive system is mapped to corresponding configuration in ZRP.

with a rate $u(n)$ that depends on the number of particles n present in the departure box (see Fig 1). The vacant sites of any particular driven diffusive system can be considered as the boxes and the domain of size n to the immediate left of this vacant site can be considered as the number of particles. Finally, the steady state current J_n can be regarded as the hop rate $u(n)$ of ZRP. Such a mapping can be shown to be exact [9] in some models. In others [6, 7], though the ZRP mapping is only approximate, phase separation could be predicted beyond doubts. Phase separation transition with $\sigma = 1,\ b > 2$ was first observed in a class of models [6] where two species of hard-core particles (equal in number) on a one-dimensional ring interact ferro-magnetically, which was extended later [7] for unequal density of particles. In these cases, b depends on the interaction strength ϵ and condensation occurs for large density of particles as ϵ is increased beyond a critical value ϵ_c. For $\epsilon < \epsilon_c$, including the antiferromagnetic interaction $\epsilon < 0$, the system remains homogeneous.

In this article we introduce a model with two species of particles which interact antiferromagnetically, where the interaction strength depends on the size of the domain. We show that such modifications can lead to phase separation transition, even for anti-ferromagnetically interacting particles. An intuitive and physical argument is provided in favour of the possibility of such a transition.

The model is defined on a ring where sites are labeled by $i = 1, 2, ...L$. Each site i can either be vacant

*E-mail address: anasuya.kundu@saha.ac.in
†E-mail address: pk.mohanty@saha.ac.in

($s_i = 0$) or occupied by a positive ($s_i = +1$) or a negative ($s_i = -1$) particle. These particles interact anti-ferromagnetically with interaction strength $\epsilon(n_l)$ which depends on the size n_l of the l^{th} block that the particles belong. Note that a block (or a *domain*) here is defined by an uninterrupted sequence of particles and leveled by an index $l = 1, 2 \ldots N_0$, where N_0 is the number of vacancies in the ring. Formally the interaction can be represented by

$$H = -\frac{1}{4}\sum_{l=1}^{N_0} \epsilon(n_l) \sum_{i \in n_l} s_i s_{i+1}. \qquad (2)$$

The model evolves according to the nearest-neighbor exchange rates

$$+- \xrightarrow{1+\Delta H} -+; \qquad +0 \xrightarrow{\alpha} 0+; \qquad 0- \xrightarrow{\alpha} -0. \quad (3)$$

Clearly, the dynamics is particle conserving. Thus the system can be characterized by the relative densities $\rho = \frac{N_+ + N_-}{N_0}$ and $\eta = \frac{N_+}{N_+ + N_-}$ where $N_\pm$ are the number of $+$ and $-$ particles respectively.

First let us consider the non-interacting case, $\epsilon = 0$. Here, the steady state weight $W(\{k_l\})$ of all the configurations in grand canonical ensemble (GCE) can be written as [6, 7]

$$W(\{n_l\}) = \prod_{l=1}^{N_0} z^{n_l} Z_{n_l}, \qquad (4)$$

where n_l is the number of particles that reside in the l^{th} block and Z_{n_l} is the sum of all microscopic configurations of a block of size n_l. The fugacity z is associated with both ($\pm$) kinds of particles. Since the weight of the configurations are factorized in terms of weight $z^{n_l} Z_{n_l}$ of individual blocks, one can draw an analogy of the model with a ZRP having N_0 boxes and $(N_+ + N_-)$ particles where steady state in GCE has a product measure; the single box weight of ZRP is $f(n) = Z_n$. Further, from the exact results of ZRP in grand canonical ensemble $f(n) = \prod_{k=1}^{n} u(k)^{-1}$, one gets $u(n) = Z_{n-1}/Z_n$ (as $Z_n = \prod_{k=1}^{n} Z_k/Z_{k-1}$). Since in the non interacting system, the current through a block of size n is $J_n = Z_{n-1}/Z_n$, one identifies $u(n) = J_n$. Now, from the assymptotic behaviour [6] of $J_n = \frac{1}{4}(1 + \frac{3/2}{n})$ one can conclude, using criteria mentioned in Eq. (1), that phase separation is not possible in this case.

The exact mapping of the model to ZRP does not hold for interacting system. However, it has been argued [6] that the correlations between neighbouring boxes can *still* be neglected for sufficiently large α and the correspondence $u(n) = J_n$ provides a correct prediction of phase separtion transition. Since the blocks are considered uncorrelated, one can calculate J_n by modeling a single block of size n where particles follow dynamics (3). Steady state weights of such a system on a ring [3] has an Ising measure $P(\{s_i = \pm\})\ \exp(-\beta H)$ with

$$H = -\frac{\epsilon}{4}\sum_i s_i s_{i+1} + h \sum_i s_i, \qquad (5)$$

i.e., weight of any configuration is same as that of the above system in equilibrium. The second term is needed to fix magnetization of the Ising system $\mathcal{M} = 2\eta - 1$. For equal density case, $h = 0$. Thus, the current

$$\begin{aligned} J_n \ &= \ \langle ++-+\rangle_n + (1-\epsilon)\langle ++--\rangle_n \\ &+ \ \langle -+--\rangle_n + (1+\epsilon)\langle -+--\rangle_n \end{aligned} \qquad (6)$$

is a static correlation function of the Ising system Eq. (5), which can be calculated [10] using the standard transfer matrix formalism [11]. For a thermodynamically large block, current J_∞ calculated on a ring is identical to that of an open domain. However, the corrections $J_n = J_\infty(1 + b(\epsilon)/n)$ depends on the boundary conditions. It has been argued [12] that $b(\epsilon)$ for an open system is related to that of the ring by a universal factor; $b(\epsilon) = \frac{3}{2} b_R$, where the subscript R stands for ring. Thus it is sufficient to calculate correlation functions Eq. (6) on a ring with respect to the equilibrium Ising measure. A simple transfer matrix formalism reveals,

$$b(\epsilon, \eta = 1/2) = \frac{3}{4}\frac{(2+\epsilon)\gamma + 2\epsilon}{\epsilon + \gamma}; \quad \gamma = \sqrt{\frac{1+\epsilon}{1-\epsilon}} + 1. \quad (7)$$

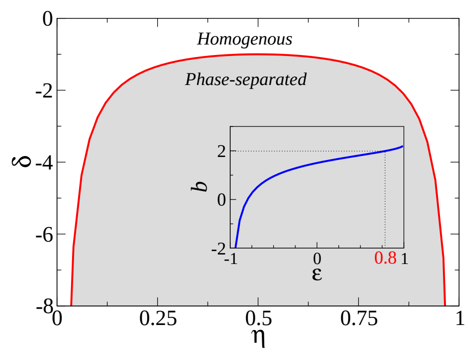

FIG. 2: Phase diagram in η-δ plane: the shaded region corresponds to phase separated state. Inset, here, shows dependence of b on ϵ for equal density case.

These relations predict that, for any relative density η the system undergoes a phase transition from a homogeneous state to a phase separated state when ϵ is increased beyond a critical threshold ϵ_c. Inset of Fig. 2 shows variation of $b(\epsilon)$ with ϵ for equal density case $\eta = 1/2$; here $\epsilon_c = 4/5$. It is evident from the figure, that phase separation is not possible when $\epsilon < 0$ (anti-ferromagnetic interaction). These predictions for ferro-magnetically interacting system have been verified using Monte Carlo simulations of extented KLS (EKLS) model for both $\eta = 1/2$ [6] and for $\eta \neq 1/2$ [7].

A possible reason, why antiferromagnetically interacting particles do not phase separate is the following. For ferro-magnetic case, each particle likes the same kind of particles as neighbours and the asymmetric exchange $+- \to -+$, then arrange more $+$ particles towards the right end of the block. With this arrangement of particles, 0s enter easily into the ferromagnetic block from

both sides allowing the movement of the whole block as a single entity. However, in an antiferromagnetic system, $+$ and $-$ particles prefer to be arranged alternatively which restrict 0s from the left (right) to move further once it encounters a $+$ $(-)$ particle. The antiferromagnetic interaction could compete with the boundary dynamics when $\epsilon \sim \mathcal{O}(1/n)$, [*i.e.* $n\epsilon \sim \mathcal{O}(\alpha)$]. Thus, it is suggestive that a phase separation could be possible when $\epsilon_n = \frac{\delta}{n}$, explicitly depends on n. In the rest of the article we concentrate on antiferromagnetic case with interaction strength $\epsilon_n = \frac{\delta}{n}$, that depends explicitly on the size of the block. It is not difficult to verify that the steady state have Ising measure. Thus, J_n can be calculated in a straightforward way following the procedure discussed here. This results in,

$$J_n \;=\; J_\infty \left(1 + \frac{3 - 4\delta J_\infty}{2n}\right); J_\infty = \eta(1-\eta). \quad (8)$$

Thus, $b(\delta, \eta) = (3 - 4\delta J_\infty)/2$ and for any given η phase separation occurs for systems having large density ρ when $\delta < -[4\eta(1-\eta)]^{-1}$. Corresponding phase diagram in η-δ plane is shown in Fig. 2.

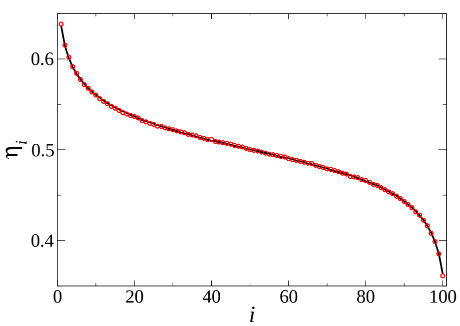

FIG. 3: Comparison of density profiles: solid line corresponds to the density profile of a block of size $n = 100$ and $L = 500$. Symbols correspond to that of a ring with 100 particles and a single defect 0. In both cases, $\delta = -0.9$.

To check the correctness of the prediction, we choose to study only the equal density case in details and verify the predictions there. In this case, $J_\infty = 1/4$ and $b(\delta) = \frac{3-\delta}{2}$; thus the transition is expected for $\delta < -1$. Note, that in deriving Eq. (8) we have assumed that, a domain containing n particles of any species, behaves like an open system where $(+)$ particles enter from left and $(-)$ particles exit from right with rate α. Hence, the dynamics of a domain can be modelled by a ring having n particles $(\pm)$ and a single defect 0, and following above dynamics. To check the validity of this assumption we have calculated the density profile of a block of size $n = 100$ using Monte Carlo simulation of a system of size $L = 500$ at $\delta = -0.9$. In Fig. 3 the density profiles of a block of size $n = 100$ obtained from Monte Carlo simulation of the full system is compared with that obtained from a ring with 100 particles and a defect 0. In both cases we choose $\delta = -0.9$. An excellent match seen here, justifies the assumption that a domain of size n in fact behaves like a ring having n particles and a single defect 0.

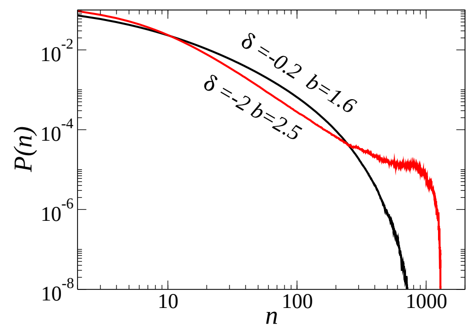

FIG. 4: Block size distribution for $\delta = -0.2$ (black) and -2.0 (red online) for a system with $L = 2000$ and $N_0 = 100$.

The coarsening dynamics of EKLS model is quite slow. Thus in fact achieving a true condensate through Monte Carlo simulations, in a finite time, is practically impossible. However, the distribution of block sizes $P(n)$, provides an indication: when $\delta < \delta_c = -1$, a condensate appears along with the usual scale-free distribution. In fact, to observe the condensate one must take the density much larger than $\rho_c = 1/(b(\delta) - 2)$. Figure 4 shows distribution of size of the block for $\delta = -0.2$ and -2.0, correspondingly the values of b are $b = 1.6$ and 2.5. The relative density is given by $\rho = 19$ with $L = 2000$. It is clear that condensation emerges only in the latter case.

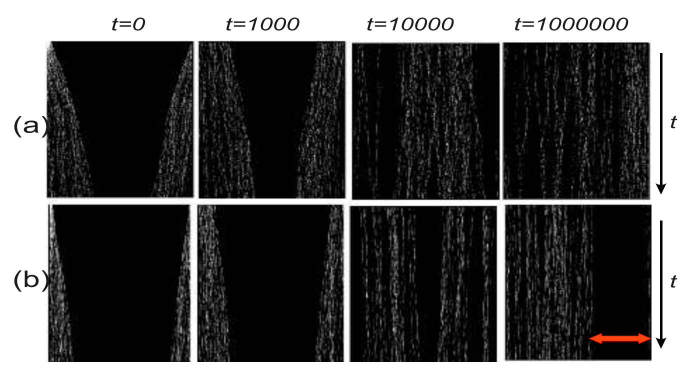

FIG. 5: Evolution of a phase separated configuration: the snapshots of the system are taken at $t = 0, 10^3, 10^4$, and 10^6. (a) Upper and (b) lower pannels correspond to $\delta = -0.2$ and -2.0 respectively. Here $L = 2000$ and $N_0 = 100$. The double arrow (red) corresponds to a large condensate that survives.

It is expected that, in the phase-separated regime, any initial phase-separated configuration evolves only to generate fluctuation in the size of the condensate; the condensate does not disappear. To check the stability of an initially phase separated configuration we have done Monte Carlo simulation of the system of size $L = 2000$ with $N_0 = 100$ and look at the space-time plots for 2000 MCS at $t = 0, 10^3, 10^4$ and 10^6. The snapshots for $\delta = -0.2$ and -2.0 are shown in Fig. 5. Clearly for

the latter case, a large condensate (indicated by a double arrow) survives even at $t = 10^6$.

In conclusion, we have studied the extended KLS model with antiferromagnetically interacting particles. The strength of interaction between particles $\epsilon(n) = \delta/n$ in this model depends explicitly on the size of the block n they belong to. The model can be mapped to zero range process by identifying vacancies as boxes; the hop rate $u(n)$ in ZRP is identified as the particle current J_n in the lattice, which can be calculated exactly. Such a mapping enables one to predict that the phase separation transition (same as condensation transition in ZRP) occurs for $\delta < -1$. These predictions are verified by using Monte Carlo simulations.

Some comments are in order. Unlike the particle current in the lattice, the hop rate in ZRP is stochastic and uncorrelated in time. Recent studies [13] of ZRP with time-correlated hop rate suggest that effective b which sets the criteria for condensation transition may change when the correlation is significantly large. However, our numerical study of the antiferromagnetic system indicates that the time-correlations, present in J_n, are possibly irrelevant. In fact, such correlations are known [9] to be irrelevant in AHR [4] model.

[1] B. Schmittmann and R.K.P. Zia, *Phase Transitions and Critical Phenomena*, vol. **17**, ed. by C. Domb and J. L. Lebowitz (Academic Press, 1995).

[2] D. Mukamel *Nonequilibrium Dynamics, Metastability and Flow*, ed. by M.E. Cates and M.R. Evans, (Institute of Physics Publishing, Bristol, 2000).

[3] S. Katz, J.L. Lebowitz, and H. Spohn, J. Stat. Phys. **34**, 497, (1984).

[4] P.F. Arndt, T. Heinzel, and V. Rittenberg, J. Phys A: Math. Gen. **31**, L45 (1998); J. Stat. Phys. 97, 1 (1999).

[5] R. Lahiri and S. Ramaswamy, Phys. Rev. Lett. **79**, 1150 (1997); R. Lahiri, M. Barma, and S. Ramaswamy, Phys. Rev. **E 61**, 1648 (2000).

[6] Y. Kafri, E. Levine, D. Mukamel, G.M. Schütz, and R.D.W. Willmann, Phys. Rev. **E 68**, 035101 (2003).

[7] M. R. Evans, E. Levine, P. K. Mohanty, D. Mukamel, Euro. Phys. J. **B 41**, 223 (2004).

[8] M. Clincy, B. Derrida, and M. R. Evans, Phys. Rev. **E 67**, 066115 (2003); A. Ayyer, E. A. Carlen, J. L. Lebowitz, P. K. Mohanty, D. Mukamel and E. R. Speer, J. Stat. Phys **137**, 1166 (2009).

[9] Y. Kafri, E. Levine, D. Mukamel, G.M. Schütz, and J. Török, Phys. Rev. Lett. **89**, 035702 (2002).

[10] J. S. Hager, J. Krug, V. Popkov, and G.M. Schutz, Phys. Rev. **E 63**, 056110 (2001).

[11] R. J. Baxter, *Exactly Solved Models in Statistical Mechanics*, (Academic Press, London, 1982).

[12] J. Krug and L. Tang, Phys. Rev. **E 50**, 104 (1994); J. Krug, Adv. Phys. **46**, 139 (1997).

[13] O. Hirschberg, D. Mukamel, and G. M. Schütz, Phys. Rev. Lett. **103**, 090602 (2009).